Techniques for using the overlap-Dirac operator to calculate hadron spectroscopy.*

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We report on our progress in using the overlap-Dirac fermion operator in simulations of lattice QCD. We have investigated the Lanczos based method of Borici, as well as various rational approximations, to calculate the step function in the overlap-Dirac operator. The QCD simulations were performed at $\beta = 5.85$ with a lattice volume of $8^3\ 32$.

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I. INTRODUCTION

The results of lattice QCD calculations of weak matrix elements are a critical component of the experimental program in heavy flavour and kaon physics. The results from lattice gauge theory calculations would significantly improve if the masses of both the sea and valence quarks could be reduced. Unfortunately progress in doing this is very slow with simulations that use either the Wilson or clover fermion operators [1].

It seems plausible that the difficulty of simulating with light quark masses with the clover and Wilson fermions operators is due to explicit chiral symmetry breaking in the actions. If the fermion operators were invariant under chiral symmetry transformations, their eigenvalue spectrum would be constrained to a smaller region [2]. The performance of the simulation algorithms degrades as the range of eigenvalues gets larger. Simulations that use the staggered fermion operator can reach much lower quark masses [1] than simulations that use the Wilson or clover operators, because the staggered action has a residual of the continuum chiral symmetry. Neuberger has derived [3] a fermion operator, called the overlap-Dirac operator, that has a lattice chiral symmetry [4, 5].

Our goal is to simulate QCD with the overlap-Dirac operator in the mass region: $(M_{PS}/M_V = 0.3 - 0.5)$. This quark mass region is inaccessible to lattice QCD simulations, that are currently computationally feasible, with the clover or Wilson operators [1].

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II. THE OVERLAP-DIRAC OPERATOR

The massive overlap-Dirac operator [3, 6] is

$$D^N = \frac{1}{2}(1+\mu+(1-\mu)\gamma_5 \frac{H(m)}{\sqrt{H(m)H(m)}}) \tag{1}$$

where $H(m)$ is the hermitian Wilson fermion operator with negative mass, defined by

$$H(m) = \gamma_5(D^W - m) \tag{2}$$

where D^W is the standard Wilson fermion operator. The parameter μ is related to the physical quark mass and lies in the range 0 to 1. The m parameter is a regulating mass, in the range between a critical value and 2.

III. NUMERICAL TECHNIQUES

Quark propagators are calculated using a sparse matrix inversion algorithm. The inner step of the inverter is the application of the fermion matrix to a vector. For computations that use the overlap-Dirac, the step function

$$\epsilon(H)\underline{b} = \frac{H}{\sqrt{HH}}\underline{b} \tag{3}$$

must be computed using some sparse matrix algorithm. A number of algorithms that calculate quark propagators from the overlap-Dirac operator, without using a nested algorithm have been proposed [7, 8]. We discuss one of them in section VI.

Practical calculations of the overlap operator are necessarily approximate. To judge the accuracy of our approximate calculation we used the (GW) Ginsparg-Wilson error:

$$|| \gamma_5 D^N \underline{x} + D^N \gamma_5 \underline{x} - 2 D^N \gamma_5 D^N \underline{x} || \frac{1}{|| \underline{x} ||} \tag{4}$$

which just checks that the matrix obeys the Ginsparg-Wilson relation [4]. Other groups [9, 10] have found that the step function must be calculated very accurately, so we also use more sophisticated estimates of the numerical error (see Eq. 8).

Our numerical simulations were done using $\beta = 5.85$ quenched gauge configurations, with a volume of 8^3 32. This allows us to directly compare our results with the two other QCD spectroscopy calculations [9, 10]. The quark propagators were generated from point sources. For all the algorithms we investigated, we used m equal to 1.5. Although we are currently investigating using the overlap-Dirac operator in the quenched theory, most of the algorithms can also be used in full QCD simulations [11, 12].

IV. LANCZOS BASED METHOD

Borici [13] has developed a method to calculate the action of the overlap-Dirac operator on a vector, using the Lanczos algorithm. In exact arithmetic, the Lanczos algorithm generates an orthonormal set of vectors that tridiagonalises the matrix.

$$HQ_n = Q_n T_n \tag{5}$$

where T_n is a tridiagonal matrix. The columns of Q_n contain the Lanczos vectors.

The "trick", to evaluate the step function (Eq. 3), is to set the target vector $\underline{b}$, as the first vector in the Lanczos sequence. An arbitrary function f of the matrix H acting on a vector is constructed using

$$\begin{aligned} (f(H)b)_i &= \sum_j (Q_n f(T_n) Q_n^\dagger)_{i\,j} b_j & (6) \\ &= \|b\| (Q_n f(T_n))_{i\,1} & (7) \end{aligned}$$

where the orthogonality of the Lanczos vectors has been used. The $f(T_n)$ matrix is computed using standard dense linear algebra routines. For the step function the eigenvalues of T_n are replaced by their moduli. Eq. 7 is linear in the Lanczos vectors and thus can be computed in two passes.

The major problem with the Lanczos procedure is the loss of the orthogonality of the sequence of vectors due to rounding errors. It is not clear how this lack of orthogonality effects the final results. Some theoretical analysis has been done on the use of the Lanczos algorithm to calculate functions of matrices [14]. It is claimed that the lack of orthogonality is not important for some classes of functions.

On small lattice we checked that the eigenvalue spectrum of the overlap-Dirac operator moves closer to a circle [15], as the number of Lanczos steps increases. Even after 50 iterations of the Lanczos algorithm, there are still small deviations from the circle. For a hot gauge configuration with a volume of 4^4, all the Lanczos vectors were stored and then were used to investigate the effect of the loss of orthogonality. The scalar product between two Lanczos vectors drops from 10^{-7} to 10^{-3} after about 130 iterations, indicating problems with orthogonality. The GW error was 0.11 at 50 iterations and 0.012 at 250 iterations. This is some evidence that the Borici's algorithm may still work even when the orthogonality of the Lanczos vectors is lost. It is much harder to look at the eigenvalue spectrum of the overlap-Dirac operator on a $8^3\ 32$ $\beta = 5.85$ gauge configuration, so we computed the GW error instead. The GW error on a single gauge configuration was: $2\ 10^{-3}$ (100 iterations), $1\ 10^{-3}$ (200) iterations, $1\ 10^{-4}$ (300) iterations, and $2\ 10^{-6}$ (500 iterations).

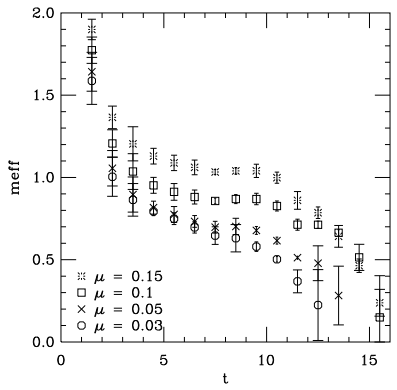

FIG. 1. Effective mass plot for pion using Borici's method of calculating the step function using 100 Lanczos iterations.

Fig. 1, is an effective mass plot of the pion, for four different values of the quark mass μ. The number of iterations in the Lanczos algorithm was kept constant at 100. The effective mass plots for the pion in Fig. 1 can be compared to the two other published spectroscopy calculations, that both use configurations with parameters: $8^3 16$ and $\beta = 5.85$. For a quark mass of $\mu = 0.1$ (0.05), Liu et al. [10] obtain a pion mass in lattice units of 0.63 (0.45). From the graph by Edwards et al. [9], the pion mass was 0.87 (0.63) at $\mu = 0.1$ (0.05). The differences between the two groups are probably explained by them using different values of m in their simulations, because the quark mass μ is renormalized by a multiplicative factor that depends on the domain mass [6]. The effective mass plots in Fig. 1 are consistent with the data of Edwards et al. [9]. Although smeared correlators should be used for a more detailed comparison. The quality of the $\mu = 0.03$ effective mass plot of the pion is disappointing. The inversion of the overlap-Dirac operator that used 100 Lanczos iterations, at a mass $\mu = 0.1$, required 150 iterations in the inverter and took 105 minutes on 32 nodes of our cray t3e.

We checked the stability of the pion's effective mass with the number of iterations used in the Lanczos procedure. The pion effective mass plot was stable for the quark masses $\mu = 0.1$ and 0.03, as the number of Lanczos iterations were varied from 100 to 300.

Liu et al. [10] used the Gell-Mann-Oakes-Renner (GOR) relation, that was derived in [6] for the overlap-Dirac operator, as a check on the accuracy of the computation of

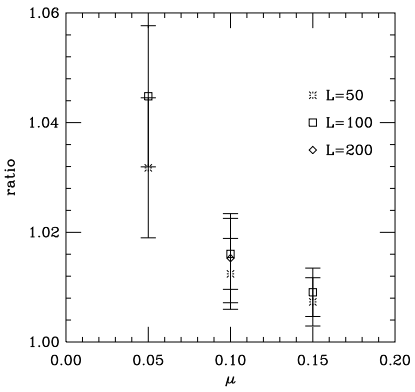

FIG. 2. The ratio of the right hand side over the left hand side in equation 8 for a single configuration. The error bars are from the Z_2 noise method used to compute the chiral condensate. The step function was computed using Borici's method with: 50, 100, 200 iterations.

the step function.

$$\mu \sum_x \langle \pi(x)\pi(0)\rangle = \frac{1}{V}\sum_x \langle \overline{\psi}(x)\psi(x)\rangle \tag{8}$$

where π is the pion interpolation field, and x is summed over the space-time volume (V). The "external" quark propagators [6] defined by

$$\hat{D}(\mu) = \frac{1}{1-\mu}[D^{-1}(\mu) - 1] \tag{9}$$

should be used in equation 8.

The data in Fig. 2 show the GOR relation is satisfied up to 2% for the masses $\mu = 0.1$ and 0.15, and 4% for the mass $\mu = 0.05$. Increasing the number of Lanczos iterations did not decrease the violation of the GOR relation. This may be due to the loss of orthogonality in the Lanczos vectors.

V. RATIONAL APPROXIMATION

The step function can be approximated by a rational approximation [16, 17].

$$\epsilon(H) \sim H\ (c_0 + \sum_{k=1}^{N} \frac{c_k}{H^2 + d_k}) \tag{10}$$

The rational approximation is only an accurate approximation to the step function in a certain region. The eigenvalues of the matrix H should lie in this region. The coefficients c_k and d_k can be obtained from the Remez algorithm [18]. The number of iterations required in the inverter is controlled by the smallest d_k coefficient, that acts like a mass. If d_k is small, the number of iterations required is controlled by the condition number of H^2.

On one configuration we obtained GW errors of: 8 10^{-5}, 1 10^{-5}, and 2 10^{-6}, for the $N = 6$, $N = 8$, and $N = 10$, optimal rational approximations [18]. Unfortunately, the above results required up to 600 iterations for the smallest d_k, which was too large to use as the inner step of a quark propagator inverter. We have not yet implemented the technique of projecting out some of the low lying eigenmodes [18]. This projection will reduce the condition number of the matrix, and hence the number of iterations required in the inner inversions.

VI. Five dimensional representation of the overlap-Dirac operator

One undesirable feature of the algorithms just presented for inverting the overlap-Dirac operator is that at each iteration of the inverter, some sparse matrix techniques must be done to calculate the overlap-Dirac operator. In the language of Krylov spaces, the theory of which underlies the numerical calculations, two independent Krylov spaces are used in a nested inverter. If the overlap-Dirac operator could be calculated using one Krylov space, this may be more efficient. Neuberger has proposed one method to calculate the overlap-Dirac operator without the nested inversion [7]. The first implementation of Neubeger's ideas was discussed by Edwards at this meeting.

To explain the idea we will use a simplified rational approximation. The generalisation to higher order rational approximations is obvious.

$$\left(\frac{1}{2}(1+\mu) + \frac{1}{2}(1-\mu)\gamma_5 c_0 H \frac{(H^2+p_1)(H^2+p_2)}{(H^2+q_1)(H^2+q_2)}\right)\psi = b \tag{11}$$

The equation for ψ can be solved using additional variables (ϕ_i). The additional equations

generated by the new variables can be written in matrix form.

$$\begin{pmatrix} -1 & 0 & 0 & 0 & H_{p1} \\ -1 & H_{q1} & 0 & 0 & 0 \\ 0 & H_{p1} & -1 & 0 & 0 \\ 0 & 0 & -1 & H_{q1} & 0 \\ 0 & 0 & 0 & \frac{1}{2}(1-\mu)\gamma_5 c_0 H & \frac{1}{2}(1+\mu) \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \psi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ b \end{pmatrix} \tag{12}$$

where we have introduced the notation $H_c = H^2 + c$.

The additional variables makes the calculation of the overlap-Dirac operator look similar to the calculation of the domain wall operator [19]. Although with an accurate enough rational approximation, this technique will calculate the overlap-Dirac operator exactly. The key issue is the condition number of the five dimensional matrix, because this controls the number of iterations required in the inverter. As the various rational approximations use small coefficients, these could have a large effect on the condition number.

To study the effect of the rational approximation on the condition number of the five dimensional matrix, we have started to study the problem in free field theory. The calculation of the eigenvalues of the matrix in Eq. 12 is simple in free field, because Fourier analysis can be used. Although the free field theory eigenvalues will not be too similar to those of the interacting theory (although projecting out the lowest topological eigenmodes will improve the agreement), this is the only case where we have any hope of analytical insight into the condition number of the five dimensional matrix.

The five dimensional matrix was constructed using MATLAB, using the free hermitian Wilson operator [20]. Table 1 contains some results for a 8^4 lattice, with a quark mass of $\mu = 0.1$, and a domain mass of $m = 1.0$. The $N16$ approximation is the 16th order approximation to the step function introduced by Neuberger and Higham [16, 17]. The $R6$, $R8$, and $R10$ rows are for the Remez approximations to the step function introduced by Edwards et al. [18]. The validity column is the maximum distance that the rational approximation deviates by 10^{-3} from unity, divided by the minimum distance. This is a measure of how good an approximation the rational function is. The order in Table 1 has been normalised so that it is comparable to the length of the lattice in the fifth dimension for domain wall fermions (the true order is obtained by multiplying by 12).

Table 1 shows that the condition number of the five dimensional matrix strongly depends on the type of rational approximation used to construct it. It is interesting to compare the $N16$ and $R8$ approximations that are almost equally good, but which

Approximation	Validity	Order	Condition number
N16	69	32	790
R6	16	13	1460
R8	61	17	2580
R10	303	21	4260

TABLE I. Condition number of the five dimensional matrix

have very different condition numbers. It would be instructive to compare the condition numbers in Table 1 with the condition number of the domain wall fermion operator [21].

VII. CONCLUSIONS

The results for the masses of the light hadrons obtained by Liu et al. [10] and Edwards et al. [9] seem to show that QCD simulations can be run at much lighter quark masses, than can be explored with the standard Wilson or clover operators. To work with quarks as light as those in the calculations of Edwards et al. and Liu et al., we need to project out the lowest eigenvalues from the H matrix. We are working on an implementation of the eigenvalue projection technique.

What is not clear is how expensive the simulations with the overlap-Dirac operator will be on more realistic lattice volumes. The only way the Wilson or clover operators can be used to simulate QCD with lighter quarks is by the brute force approach of simulating closer to the continuum limit. This too will be very expensive. As the overlap-Dirac operator has a lattice chiral symmetry, it should be able to be used to explore the light quark mass region of QCD in an elegant way.

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